DIESEL COMBUSTION/EMISSIONS RESEARCH

Dennis L. Siebers
Sandia National Laboratories
Livermore, CA 94550

Introduction

In collaboration with industry, the DOE Office of Heavy Vehicle Technology (OHVT) is conducting an ambitious program to significantly increase the efficiency, reduce the emissions, and improve the fuel-flexibility of heavy-duty diesel engines. This program, the Low Emission Diesel (LE-55) program, is targeting a production heavy-duty diesel engine by 2002 with an efficiency of 55% and NOx and particulate emissions of 2 gm/HP-hr and 0.05 gm/HP-hr, respectively. Current heavy-duty diesel engines have thermal efficiencies of 44%, with NOx and particulate emissions just under 5 gm/HP-hr and 0.1 gm/HP-hr, respectively. The overall goal of this program is to help U.S. efforts to reduce its dependence on imported petroleum, improve air quality, and enhance economic growth and the competitiveness of U.S. industry.

Achieving the LE-55 targets will require significant improvements in many areas of diesel engine technology. One critical area will be the design of the injection/combustion system and the associated control of emissions in-cylinder. Much of the progress already made on diesel combustion and emissions has been achieved with an iterative "trail and error" approach that has been costly, time consuming, and as a result, limited to directions within the present "experience base" of industry. The uncertainty and cost associated with this method of improvement, however, will inhibit the innovation and progress on diesel engine combustion system design that is needed to achieve the LE-55 targets. A new design approach is required; one guided by a more complete understanding of diesel combustion and emissions processes and validated comprehensive combustion system design tools (*i.e.*, multidimensional computational fluid dynamics and chemical kinetics models) that embody that new understanding. Such an approach will speed the diesel engine development and optimization process and foster new and innovative concepts for helping meet the LE-55 targets.

The following briefly summarizes recent experimental research and model development efforts aimed at improving our understanding of diesel combustion and emissions processes and developing combustion system design tools. The work has been conducted at Sandia, Los Alamos, and Lawrence Livermore National Laboratories. In addition, future research directions are briefly discussed, including a new experimental research effort on alternative fuels for diesels.

The emphasis in the following discussion is on the experimental research which was partially supported by OHVT in the past year and will be fully supported by OHVT over the next three years through a new CRADA being developed with diesel engine manufacturers. The model development efforts discussed will also be covered under the new CRADA starting in FY98, but are presently funded through other DOE Defense Program or Energy and Efficiency projects.

Investigations of Diesel Injection, Combustion and Emissions Processes

Experimental research aimed at developing a new and more comprehensive understanding of in-cylinder diesel injection, combustion and emissions processes is being conducted at Sandia National Laboratories in collaboration with industry. The goal has been to utilize new advanced laser based diagnostics to determine the structure of a diesel jet, how this structure is controlled by and scales with various parameters, and the evolution of the combustion and emissions formation processes.

The research is being conducted in two facilities: a diesel engine facility and a recently completed diesel combustion simulation facility. The diesel engine facility consists of a single-cylinder, Cummins diesel engine with extensive optical access. The engine is characteristic of on-highway heavy-duty truck engines. The diesel simulation facility consists of a pressure vessel with complete optical access in which diesel engine conditions can be simulated over a much wider range of conditions than is possible in an engine. Conditions that can be simulated include high power density conditions with peak combustion pressures more than a factor of two higher than in present diesel engines.

The results from these experiments are providing engine designers with new insights and are being used to help develop and validate computer models of in-cylinder diesel engine processes (*i.e.*, KIVA). Some recent key results are:

- The in-cylinder gas density has been found to have a larger effect on the penetration of diesel jets than previously noted. This effect is caused by a dependence of penetration on the dispersion of a diesel jet, an effect that is not accounted for in common models for penetration. Penetration time and length scales have been developed that account for this effect and that correlate penetration data over an extremely wide range of conditions.
- Penetration is affected by fuel vaporization and combustion with vaporization reducing penetration by as much as 20% and combustion increasing it by 30-40%.
- Liquid fuel in a diesel jet is confined to a narrow, short region extending only 20-30 mm from the injector tip for typical diesel engine conditions. This region is much smaller than previous conceptual models of diesel jets indicate or current multi-dimensional models predict.
- After ignition and the initial premixed burn, a portion of the fuel is believed to continuously burn in a rich premixed flame located near the tip of the liquid region. (The existence of the rich premixed flame has been inferred from various measurements.) The remaining fuel burns in a diffusion flame zone surrounding the entire jet region downstream of the liquid region. This diffusion flame zone is thin but can be highly distorted by turbulence.
- Soot formation occurs in a progressive manner beginning just downstream of the liquid-fuel zone, most likely in the rich premixed flame region. In this region, the soot concentration is low and the soot particle size is small. Progressing toward the leading edge of the jet, the concentration of soot particles and the particle size increase.

In the coming year, the experimental research will focus on determining the evolution of NO in a diesel jet and the parameters that control the extent of the liquid phase in a diesel jet. This research will be supported by DOE's OHVT under a new CRADA with the diesel engine industry. In addition, a new experimental project supporting the development of a fuel-flexible diesel engine will begin. This fuels research will focus on using the advanced laser-

based diagnostics to understand the effects of various alternative fuels (*e.g.*, biodiesel, alcohols, gasoline and blends of these fuels with diesel fuel) on diesel combustion and emissions formation processes. A new state-of-the-art optical access diesel engine will be built for the alternative fuels research.

Computational Fluid Dynamics Model Developments

Multidimensional computational fluid dynamics (CFD) models for in-cylinder diesel engine flow, spray, combustion, and emissions processes are being developed at Los Alamos National Laboratory. This project has resulted in the widely used KIVA code for engine combustion simulations. KIVA solves the equations for turbulent, chemically reactive flow with sprays in three dimensions. The numerical method utilizes a computational mesh of arbitrary hexahedra that can conform to complex boundary shapes and follow the motion of pistons and valves. The latest version of the code, KIVA-3, uses a block structured mesh to calculate coupled port and in-cylinder flows. Largely because of KIVA, three-dimensional calculations with sprays and/or combustion have become common place in the engine design process.

The recent focus of the CFD work has been on developing a next generation code for engine combustion and emissions processes. This code, which is called CHAD (Computational Hydrodynamics for Advanced Design), is being developed to meet the expanded needs of the engine industry for integrating more detailed and accurate hydrodynamics calculations into the engine design process. (In addition to predicting in-cylinder combustion and emissions processes, however, CHAD can be applied to external aerodynamics and under-hood cooling problems.)

CHAD improves on current codes for engine design in three ways. First, it is written in a highly scaleable and portable manner to deliver desktop to multiple gigaflop performance on existing massively parallel computer architectures. The code is portable to uniprocessor workstations, symmetric multiprocessors, clusters of workstations, and massively parallel platforms. Because communication systems are not standardized and are changing rapidly, all communication coding is isolated into a locally developed portable library. CHAD's second improvement is that it utilizes an unstructured computational mesh of hexahedra and degenerate elements derived from hexahedra - including tetrahedra, prisms, and pyramids. This geometric flexibility will ease mesh generation problems and allow meshes with less element distortion, and consequently calculations with less numerical error. The third improvement is the use of a novel variable explicit/implicit multidimensional convection method that automatically uses an accurate explicit method where and when this is possible and switches locally and continuously to an implicit method when necessary.

Recent progress on CHAD includes the incorporation of a new edge-based data structure that greatly improves computational efficiency, development of a portable message-passing library, and incorporation of multiple species transport and finite-rate chemistry. The portable message passing library is expected to give scaleable performance on shared- and distributed-memory parallel computer architectures.

In the coming year, the CFD model work related to diesel engines will focus on developing a new spray model for KIVA and CHAD and comparing the overall model predictions with the new experimental results. The spray model is the only major submodel that is lacking for diesel applications of CHAD.

Computational Chemical Kinetics Model Developments

Computational models that describe the chemical reactions of hydrocarbon fuels in compression ignition engines are being developed at Lawrence Livermore National Laboratory. These models simulate the overall combustion chemistry of fuels, as well as the chemistry leading to oxides of nitrogen (NOx) and soot emissions. They are intended to be used in a standalone mode to study the details of chemical processes, or they can be used to develop simplified kinetics submodels for use in the multidimensional CFD models of diesel combustion (*e.g.*, CHAD and KIVA). The CFD models can then be used to assist in engine design work, with the simplified chemical kinetics submodels providing reliable predictions of the fuel chemistry and the major emissions, particularly soot and NOx.

The current focus of this work is on using the detailed chemistry models to help develop an understanding of the details of the soot and NOx production chemistry. The soot studies are concentrating on the early chemical pathways leading to soot formation. These chemical paths involve formation of species containing single and multiple aromatic rings. These detailed chemical kinetic models are beginning to provide an understanding of some of the key reaction steps in these soot precursor pathways. Future detailed chemical kinetics investigations will focus on the kinetics and the thermochemistry of simple aromatic compounds and the smaller C_3 and C_4 species that appear to produce aromatic species. The goal is to build a more complete model for species growth leading to the eventual soot particle production.

Investigations using detailed kinetics models to explore NOx formation issues are also planned. Production of NOx in diesel engines is primarily the result of the Zeldovich reaction mechanism involving oxygen and nitrogen which is particularly rapid at high temperatures. However, hydrocarbon chemistry interacts with production of NOx in many complex ways. Under some conditions, hydrocarbon oxidation reactions can convert NO to NO_2 and complicate the chemical processes and the models needed to provide accurate computer simulations of NOx emissions.